Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.81e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.91e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
Tribromoacetic acid	Dibromoacetic acid	4-Hydroxybenzoic acid
Measured: 6.74e-01	**Measured:** 9.69	**Measured:** 3.62e-02
Predicted: 5.34e-01	**Predicted:** 4.01	**Predicted:** 9.91e-02